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Characteristics

Classification

Compound

Authors

1 MANDELATE RACEMASE MUTANT D: CO-CRYSTALLIZED WITH (S)- ATROLACTATE

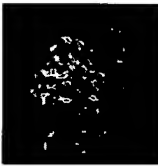
Release Date: 14-Oct-1996 Exp. Method:

Resolution: 2.10 Å

Racemase

Mol. Id: 1 Molecule: Mandelate Racemase

Mutation: E317Q

Mitra, B., Kallarakal, A.T., Kozarich
J.A., Clifton, J.G., Petsko, G.A., Kei☒ 1B73

Characteristics

Classification

Compound

Authors

GLUTAMATE RACEMASE FROM AQU: PYROPHILUS

Release Date: 28-Jan-1999 Exp. Method:

Resolution: 2.30 Å

Isomerase

Mol. Id: 1 Molecule: Glutamate Racemase

Hwang, K.Y., Cho, C.S., Kim, S.S.,
H.C., Yu, Y.G., Cho, Y.☒ 1B74

Characteristics

Classification

Compound

Authors

GLUTAMATE RACEMASE FROM AQU: PYROPHILUS

Release Date: 28-Jan-2000 Exp. Method:

Resolution: 2.30 Å

Isomerase

Mol. Id: 1 Molecule: Glutamate Racemase

Hwang, K.Y., Cho, C.S., Kim, S.S.,
H.C., Yu, Y.G., Cho, Y.☒ 1ZUW

Characteristics

Classification

Compound

Authors

Crystal structure of B.subtilis gluta racemase (Race) with D-Glu

Release Date: 06-Dec-2005 Exp. Method:

Resolution: 1.75 Å

Isomerase

Mol. Id: 1 Molecule: Glutamate Racemase

Ruzheinikov, S.N., Taal, M.A., Sede
S.E., Baker, P.J., Rice, D.W.

1

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#23 Search #21 AND crystal	14:27:36	3
#30 Related Articles for PubMed (Select 10331867)	14:27:32	132
#29 Related Articles for PubMed (Select 10089337)	14:27:20	296
#28 Search #27 AND #26 AND #21	14:27:07	0
#27 Search crystal or x-ray or "x ray" or diffraction	14:26:49	797671
#26 Search "Helicobacter pylori"[MeSH]	14:26:19	18826
#22 Search #21 AND pylori	14:11:21	1
#21 Search "glutamate racemase"[Substance Name]	14:11:03	48

Clear History

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Apr 4 2006 06:32:46

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☐ 1: **glutamate racemase [Substance Name]**
catalyzes the conversion of L-glutamate to D-glutamate
Date introduced: February 8, 1990

Registry Number: EC 5.1.1.3

Heading Mapped to:

- [Amino Acid Isomerases](#)

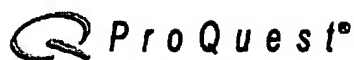
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| 2. ("glutamate racemase" OR Murl) AND crystal
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E "GLUTAMATE RACEMASE"/CN 25

L1 1 S E3

FILE 'MEDLINE, AGRICOLA, CAPLUS, BIOSIS, EMBASE, WPIDS' ENTERED AT
14:35:29 ON 07 APR 2006

L2 5858 S L1 OR MURI!

L3 20 S L2 AND PYLORI

L4 1 S L3 AND CRYSTAL

L5 29 S L2 AND (CRYSTAL OR DIFFRACT? OR X-RAY OR (X (W) RAY))

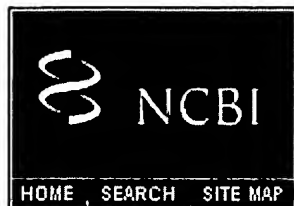
L6 20 DUP REM L5 (9 DUPLICATES REMOVED)

L7 4 S L6 AND PYLORI

L8 16 S L6 NOT L7

FILE 'STNGUIDE' ENTERED AT 14:44:40 ON 07 APR 2006

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[gi: 11133705]

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Structure

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1B74 A



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1ZUH C



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(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
22 July 2004 (22.07.2004)

PCT

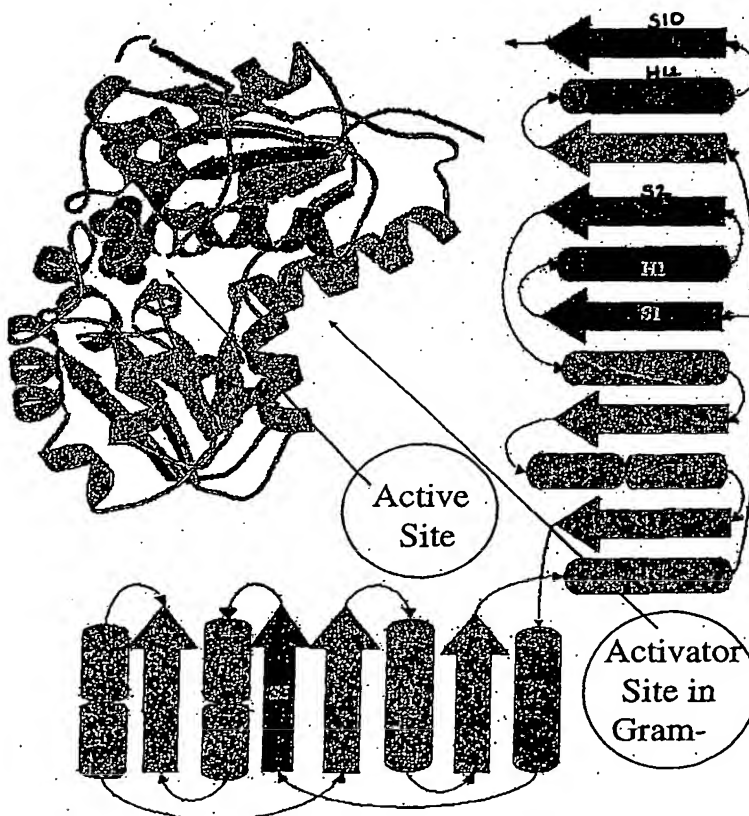
(10) International Publication Number
WO 2004/061097 A3

- (51) International Patent Classification⁷: C12N 9/90, (72) Inventors; and
15/61, G01N 33/573 (75) Inventors/Applicants (for US only): ANDERSON, Marie [GB/SE]; Styrsvägem 18, SE-437 93 Lindome (SE). FISHER, Stewart, Lindsay [US/US]; 18 Harrington Road, Framingham, MA 01701 (US). FOLMER, Rutger, Henk, Adriaan [NL/SE]; Bräckavägen 45, 437 42 Lindome (SE). KERN, Gunther [DE/US]; 71 Ravenswood Road, Waltham, MA 02453 (US). LUNDQVIST, Rolf, Tomas [SE/SE]; Övre Djupedalsgatan 9c, SE-413 07 Gothenburg (SE). NEWTON, David, Trevor [CA/CA]; 696 Mathieu Way, Ottawa, Ontario K4A 2S4 (CA). XUE, Yafeng [CN/SE]; Askims svedjev. 24, SE-436 42 Askim (SE).
- (21) International Application Number: PCT/US2003/038977
- (22) International Filing Date: 8 December 2003 (08.12.2003)
- (25) Filing Language: English
- (26) Publication Language: English
- (30) Priority Data:
60/435,167 20 December 2002 (20.12.2002) US
60/435,272 20 December 2002 (20.12.2002) US
60/435,087 20 December 2002 (20.12.2002) US
60/435,527 20 December 2002 (20.12.2002) US
- (71) Applicants (for all designated States except US): ASTRAZENECA AB [SE/SE]; S-151 85 Södertälje (SE). ASTRAZENECA PHARMACEUTICALS LP [US/US]; 1800 Concord Pike, Wilmington, DE 19850-5438 (US).
- (74) Agents: PHILLIPS, Neil, Godfrey, Alasdair et al.; Astrazeneca AB, Global Intellectual Property, SE-151 85 Södertälje (SE).
- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR,

[Continued on next page]

(54) Title: CRYSTAL STRUCTURE OF GLUTAMATE RACEMASE (MUR)

Topology diagram of MurI



(57) Abstract: The present invention discloses crystals of MurI from Gram negative, Gram positive, and atypical bacterium; computer-assisted method for screening, identifying, and designing inhibitors of MurI; inhibitors of MurI; and uses thereof.

WO 2004/061097 A3



CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

- (84) Designated States (*regional*): ARIPO patent (BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments

- (88) Date of publication of the international search report:

23 September 2004

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INTERNATIONAL SEARCH REPORT

International Application No

PCT/US 03/38977

A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C12N9/90 C12N15/61 G01N33/573

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C12N G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, BIOSIS, Sequence Search, EMBL, EMBASE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	HWANG KWANG YEON ET AL: "Structure and mechanism of glutamate racemase from Aquifex pyrophilus" NATURE STRUCTURAL BIOLOGY, vol. 6, no. 5, May 1999 (1999-05), pages 422-426, XP002286544 ISSN: 1072-8368 cited in the application the whole document ----- -/--	1-40, 45-47

☒ Further documents are listed in the continuation of box C.☒ Patent family members are listed in annex.

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Date of the actual completion of the International search

1 July 2004

Date of mailing of the International search report

15/07/2004

Name and mailing address of the ISA

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INTERNATIONAL SEARCH REPORT

International Application No

PCT/US 03/38977

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	HWANG KWANG YEON ET AL: "Crystallization and preliminary X-ray analysis of glutamate racemase from Aquifex pyrophilus, a hyperthermophilic bacterium" ACTA CRYSTALLOGRAPHICA SECTION D BIOLOGICAL CRYSTALLOGRAPHY, vol. 55, no. 4, April 1999 (1999-04), pages 927-928, XP008031528 ISSN: 0907-4449 the whole document	1-40, 45-47
X	DE DIOS ALFONSO ET AL: "4-substituted D-glutamic acid analogues: The first potent inhibitors of glutamate racemase (MurI) enzyme with antibacterial activity" JOURNAL OF MEDICINAL CHEMISTRY, vol. 45, no. 20, 26 September 2002 (2002-09-26), pages 4559-4570, XP002286546 ISSN: 0022-2623 the whole document	36-40, 45-47
X	WO 02/14261 A (TEBBE MARK JOSEPH ; MARTIN JOSE ALFREDO (ES); DIOS ALFONSO DE (ES); PR) 21 February 2002 (2002-02-21) the whole document	36-40, 45-47
X	GLAVAS S ET AL: "The inhibition of glutamate racemase by d-N-hydroxyglutamate" BIOORGANIC & MEDICINAL CHEMISTRY LETTERS, OXFORD, GB, vol. 7, no. 17, 9 September 1997 (1997-09-09), pages 2265-2270, XP004136426 ISSN: 0960-894X the whole document	45-47
X	KIM WOO-CHANG ET AL: "Isolation of peptide ligands that inhibit glutamate racemase activity from a random phage display library" JOURNAL OF BIOMOLECULAR SCREENING, vol. 5, no. 6, December 2000 (2000-12), pages 435-440, XP008032389 ISSN: 1087-0571 the whole document	45-47

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INTERNATIONAL SEARCH REPORT

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PCT/US 03/38977

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Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	TANNER MARTIN E ET AL: "The synthesis and stability of aziridino-glutamate, an irreversible inhibitor of glutamate racemase" TETRAHEDRON LETTERS, vol. 35, no. 24, 1994, pages 4073-4076, XP002286565 ISSN: 0040-4039 the whole document -----	45-47
A	GLAVAS SUZANA ET AL: "Active site residues of glutamate racemase" BIOCHEMISTRY, vol. 40, no. 21, 29 May 2001 (2001-05-29), pages 6199-6204, XP002286547 ISSN: 0006-2960 the whole document -----	1-40, 45-47
A	PUCCI M J ET AL: "THE ESCHERICHIA COLI DGA (MURI) PROTEIN SHARES BIOLOGICAL ACTIVITY AND STRUCTURAL DOMAINS WITH THE PEDIOCOCCUS PENTOSACEUS GLUTAMATE RACEMASE" JOURNAL OF BACTERIOLOGY, WASHINGTON, DC, US, vol. 176, no. 2, January 1994 (1994-01), pages 528-530, XP001035226 ISSN: 0021-9193 the whole document -----	1-40, 45-47

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US 03/38977

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☒ Claims Nos.: 41-44
because they relate to subject matter not required to be searched by this Authority, namely:
Although claims 45 and 46 are directed to a method of treatment of the human/animal body, the search has been carried out and based on the alleged effects of the compound/composition.
2. ☐ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this International application, as follows:

see additional sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☒ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐ The additional search fees were accompanied by the applicant's protest.

☐ No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Although claims 45 and 46 are directed to a method of treatment of the human/animal body, the search has been carried out and based on the alleged effects of the compound/composition.

Continuation of Box I.1

Claims Nos.: 41-44

The subject matter of claims 41 to 44 has not been searched, since it falls under the provisions of Rule 39.1(iii) PCT (Scheme, rules and method for doing business).

Information on patent family members

PCT/US 03/38977

Form PCT/ISA/210 (patent family annex) (January 2004)